

Lattice Computations for High Energy and Nuclear Physics

Karl Jansen



- **Progress in Lattice Field Theory computations**
- **The lattice and the Higgs boson**
- **Selected results from lattice QCD simulations**
 - Baryon spectrum
 - The anomalous magnetic moment of the muon
- **Challenges**
 - Nucleon structure, light-by-light scattering
⇒ simulations at physical pion masses
- **New directions**
 - Nuclear physics
 - Search for the conformal window
- **Conclusion**

Schwinger model: 2-dimensional Quantum Electrodynamics

(Schwinger 1962)

Quantization via Feynman path integral

$$\mathcal{Z} = \int \mathcal{D}A_\mu \mathcal{D}\Psi \mathcal{D}\bar{\Psi} e^{-S_{\text{gauge}} - S_{\text{ferm}}}$$

Fermion action

$$S_{\text{ferm}} = \int d^2x \bar{\Psi}(x) [D_\mu + m] \Psi(x)$$

gauge covariant derivative

$$D_\mu \Psi(x) \equiv (\partial_\mu - ig_0 A_\mu(x)) \Psi(x)$$

with A_μ gauge potential, g_0 bare coupling

$$S_{\text{gauge}} = \int d^2x F_{\mu\nu} F_{\mu\nu}, \quad F_{\mu\nu}(x) = \partial_\mu A_\nu(x) - \partial_\nu A_\mu(x)$$

equations of motion: obtain classical **Maxwell equations**

Lattice Schwinger model

introduce a **2-dimensional** lattice with
lattice spacing a

fields $\Psi(x)$, $\bar{\Psi}(x)$ on the lattice sites

$x = (t, \mathbf{x})$ integers

discretized fermion action

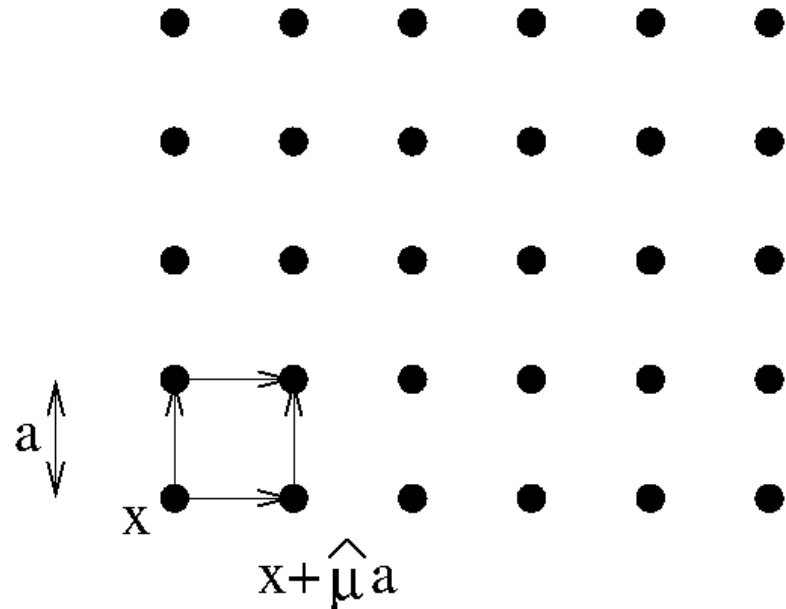
$$S \rightarrow a^2 \sum_x \bar{\Psi} [\gamma_\mu \partial_\mu - r \underbrace{\partial_\mu^2}_{\nabla_\mu^* \nabla_\mu} + m] \Psi(x)$$

$$\partial_\mu = \frac{1}{2} [\nabla_\mu^* + \nabla_\mu]$$

discrete derivatives

$$\nabla_\mu \Psi(x) = \frac{1}{a} [\Psi(x + a\hat{\mu}) - \Psi(x)] , \quad \nabla_\mu^* \Psi(x) = \frac{1}{a} [\Psi(x) - \Psi(x - a\hat{\mu})]$$

second order derivative \rightarrow remove doubler \leftarrow break chiral symmetry

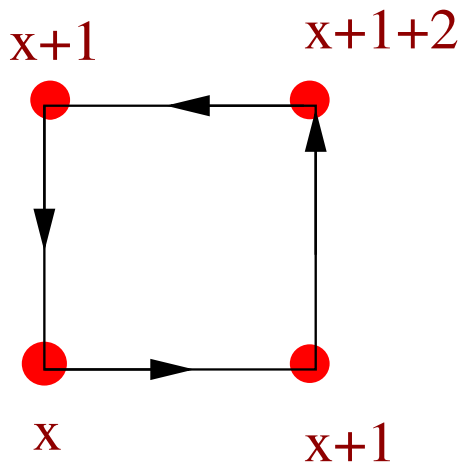


Implementing gauge invariance

Wilson's fundamental observation: introduce Paralleltransporter connecting the points x and $y = x + a\hat{\mu}$:

$$U(x, \mu) = e^{iaA_\mu(x)} \in U(1)$$

$$\Rightarrow \text{lattice derivative: } \nabla_\mu \Psi(x) = \frac{1}{a} [U(x, \mu)\Psi(x + \mu) - \Psi(x)]$$



$$U_p = U(x, \mu)U(x + \mu, \nu)U^\dagger(x + \nu, \mu)U^\dagger(x, \nu)$$

$$\rightarrow F_{\mu\nu}F^{\mu\nu}(x) \quad \text{for } a \rightarrow 0$$

$$S = a^2 \sum_x \left\{ \beta [1 - \text{Re}(U_{(x,p)})] + \bar{\psi} \left[m_0 + \frac{1}{2} \{ \gamma_\mu (\nabla_\mu + \nabla_\mu^*) - a \nabla_\mu^* \nabla_\mu \} \right] \psi \right\}$$

Partition functions (pathintegral) with Boltzmann weight (action) S

$$\mathcal{Z} = \int_{\text{fields}} e^{-S}$$

Physical Observables

expectation value of physical observables \mathcal{O}

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int_{\text{fields}} \mathcal{O} e^{-S}$$

↓ lattice discretization

01011100011100011110011

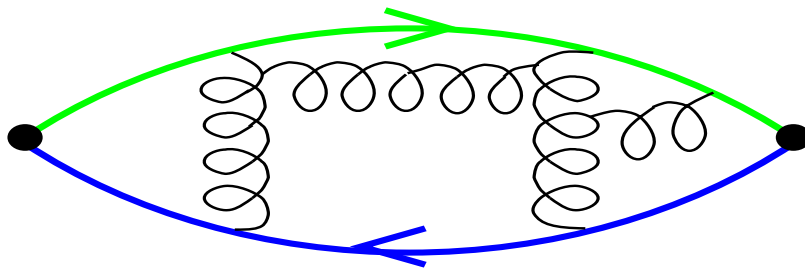
↓



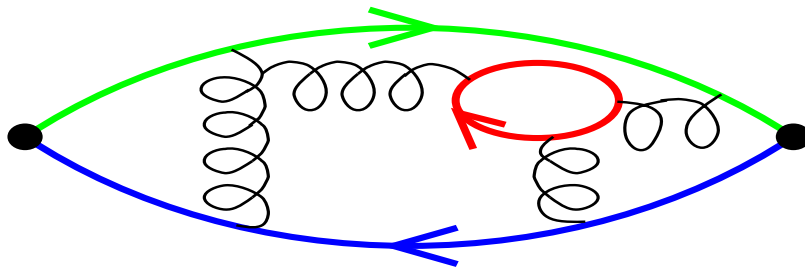
Lattice Field Theory in the 20th century: the Quenched Approximation

→ neglect internal quark-antiquark loops antiquarks in physical quantum processes

⇒ severe *truncation*



(A) Quenched QCD: no internal quark loops

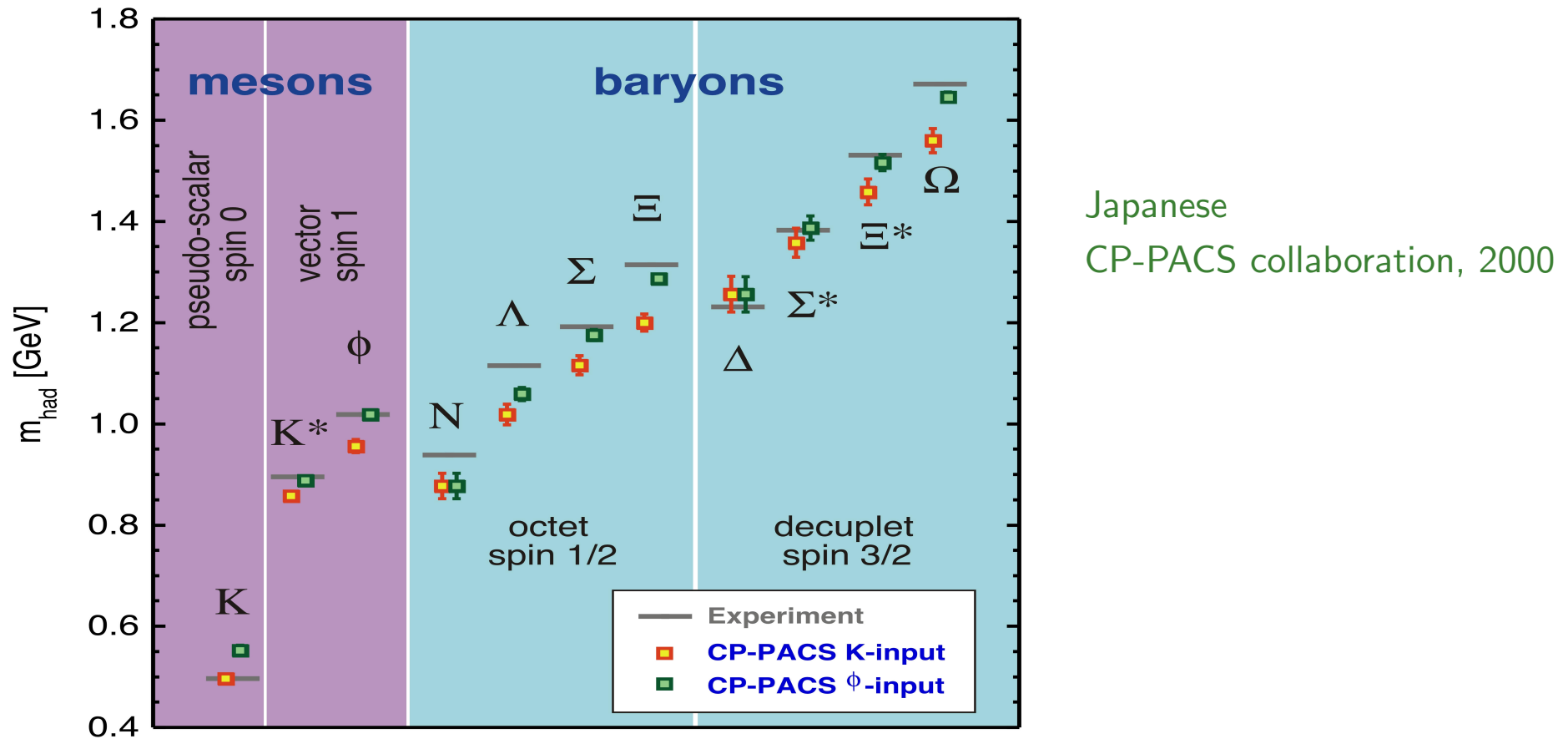


(B) full QCD

Quenched approximation



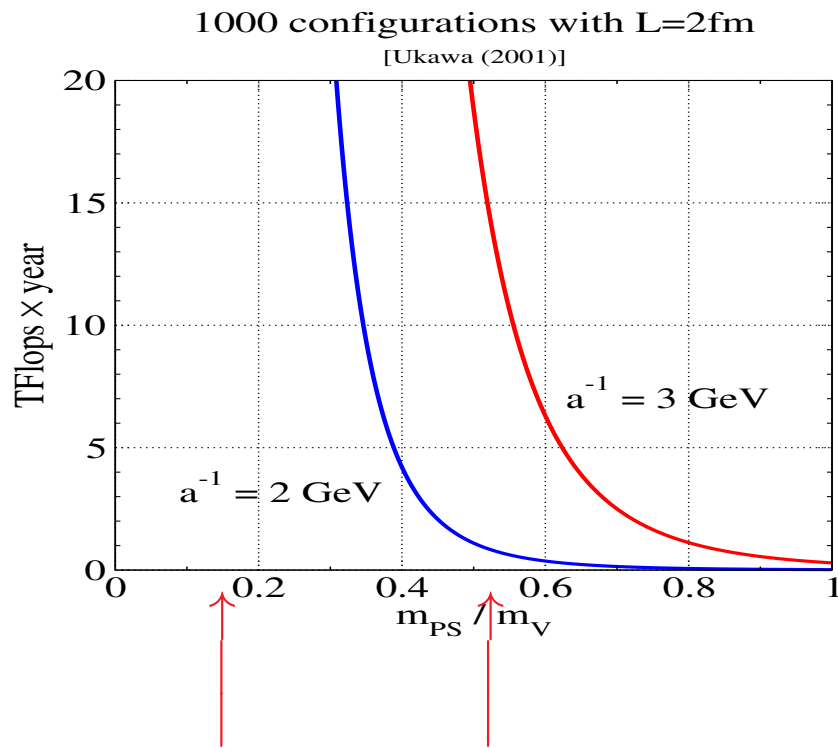
Status in 2000: neglecting internal quark loops



End of the “quenched area”: need to take quark loops into account

Costs of dynamical fermions simulations, the “Berlin Wall”

see panel discussion in Lattice2001, Berlin, 2001



physical
point

contact to
 χ PT (?)

$$\text{formula } C \propto \left(\frac{m_\pi}{m_\rho} \right)^{-z_\pi} (L)^{z_L} (a)^{-z_a}$$

$$z_\pi = 6, \quad z_L = 5, \quad z_a = 7$$

“both a 10^8 increase in computing power AND spectacular algorithmic advances before a useful interaction with experiments starts taking place.”

(Wilson, 1989)

⇒ need of **Exaflops Computers**

Why are fermions so expensive?

- need to evaluate

$$\mathcal{Z} = \int \mathcal{D}\bar{\psi} \mathcal{D}\psi e^{-\bar{\psi} \{D_{\text{lattice}}^{\text{Dirac}}\} \psi} \propto \det[D_{\text{lattice}}^{\text{Dirac}}]$$

- bosonic representation of determinant

$$\det[D_{\text{lattice}}^{\text{Dirac}}] \propto \int \mathcal{D}\Phi^\dagger \mathcal{D}\Phi e^{-\Phi^\dagger \{D_{\text{lattice}}^{-1}\} \Phi}$$

- need vector $X = D_{\text{lattice}}^{-1} \Phi$

- solve linear equation $D_{\text{lattice}} X = \Phi$

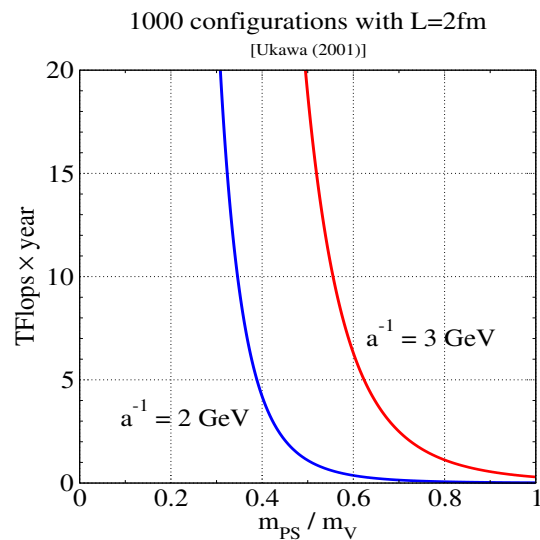
D_{lattice} matrix of dimension 100million \otimes 100million $\approx 12 \cdot 48^3 \cdot 96$
(however, matrix is sparse)

- number of such “inversions”: $O(100 - 1000)$ for one field configuration
- want: $O(1000 - 10000)$ such field configurations

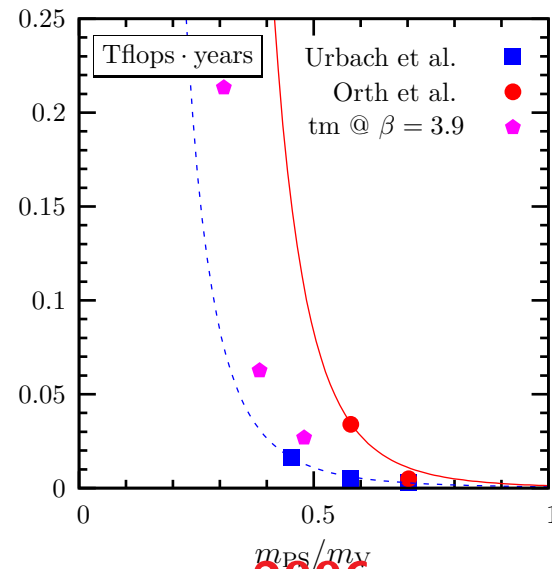
A generic improvement for Wilson type fermions

New variant of HMC algorithm (Urbach, Shindler, Wenger, K.J.)
(see also SAP (Lüscher) and RHMC (Clark and Kennedy) algorithms)

- even/odd preconditioning
- (twisted) mass-shift (Hasenbusch trick)
- multiple time steps



2001

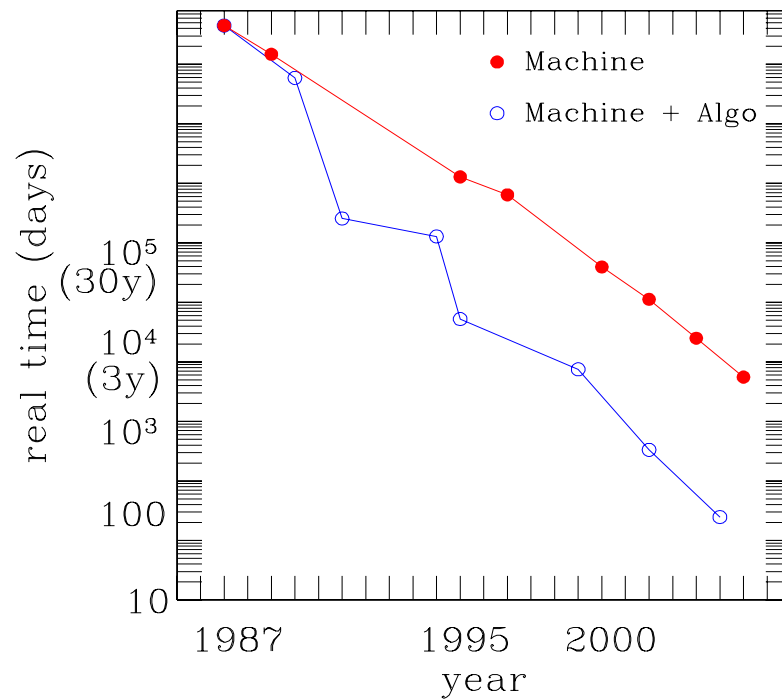


2006

- comparable to staggered
- reach small pseudo scalar masses $\approx 300\text{MeV}$

Computer and algorithm development over the years

time estimates for simulating $32^3 \cdot 64$ lattice, 5000 configurations

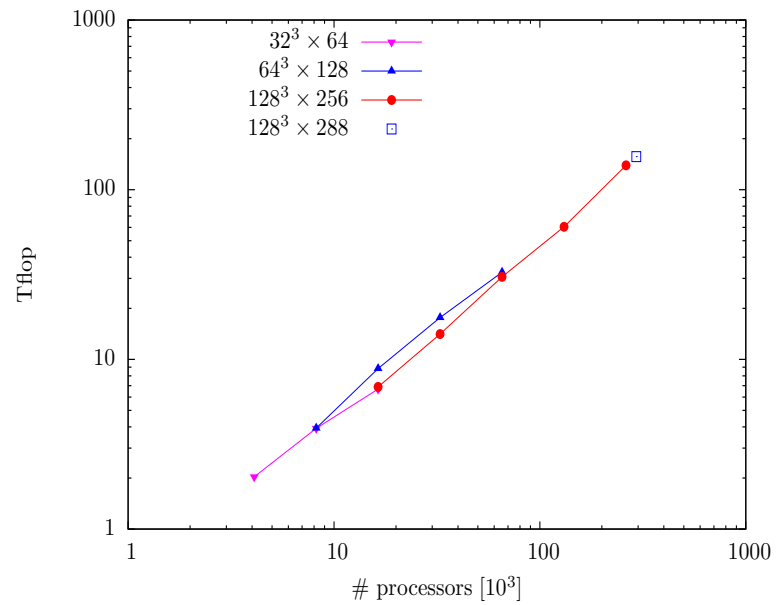


→ algorithm development very important

→ typical architectures: **BG/L,P,Q, GPUs**

Strong Scaling

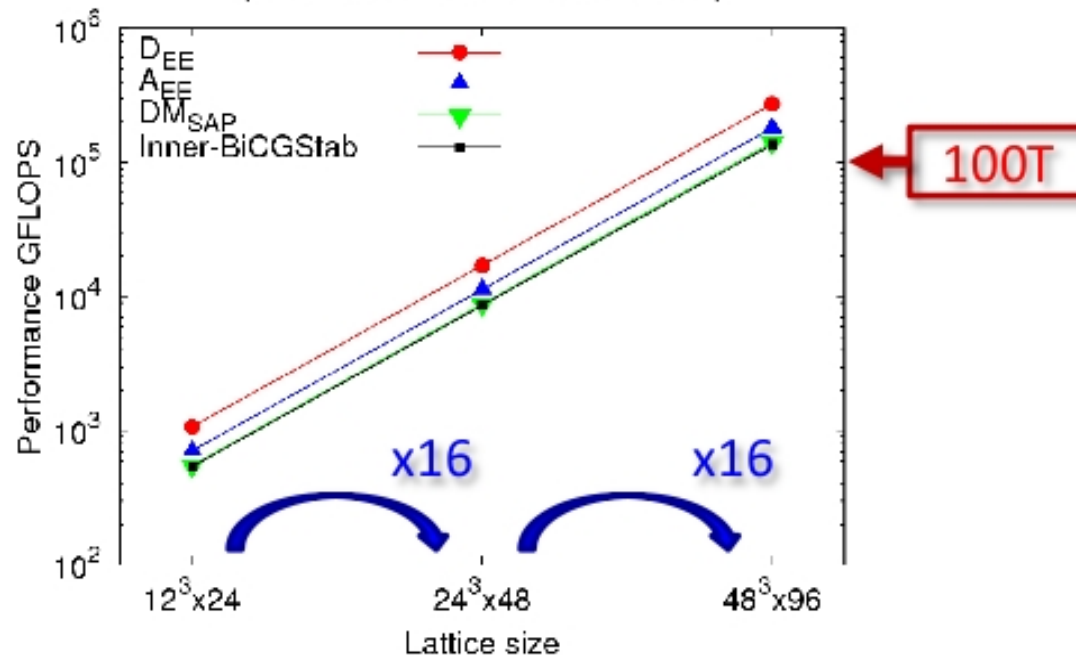
- Test on 72 racks BG/P installation at supercomputer center Jülich (Gerhold, Herdioza, Urbach, K.J.)
- using tmHMC code



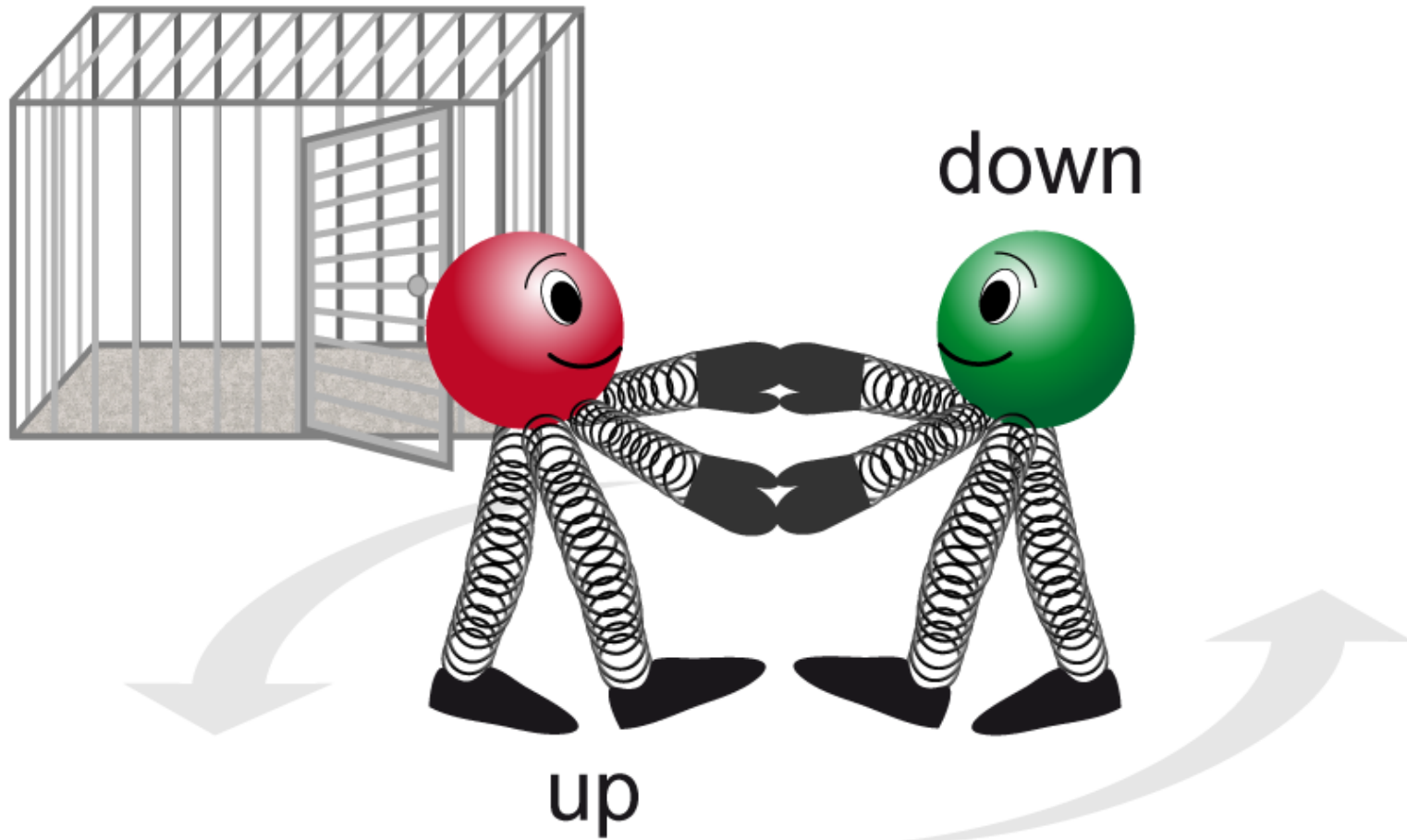
Lattice QCD code on the K-computer: weak scaling

(K. Ishikawa in collaboration with T.Boku, Y.Kuramasi, K.Minami, Y.Nakamura, F.Shoji, D.Takahashi, M.Terai, A.Ukawa, T.Yoshie (RIKEN-Tsukuba Joint Research))

Weak scaling sustained performance of the single precision kerr
(block size = 6^4 , 2-blocks in a node).

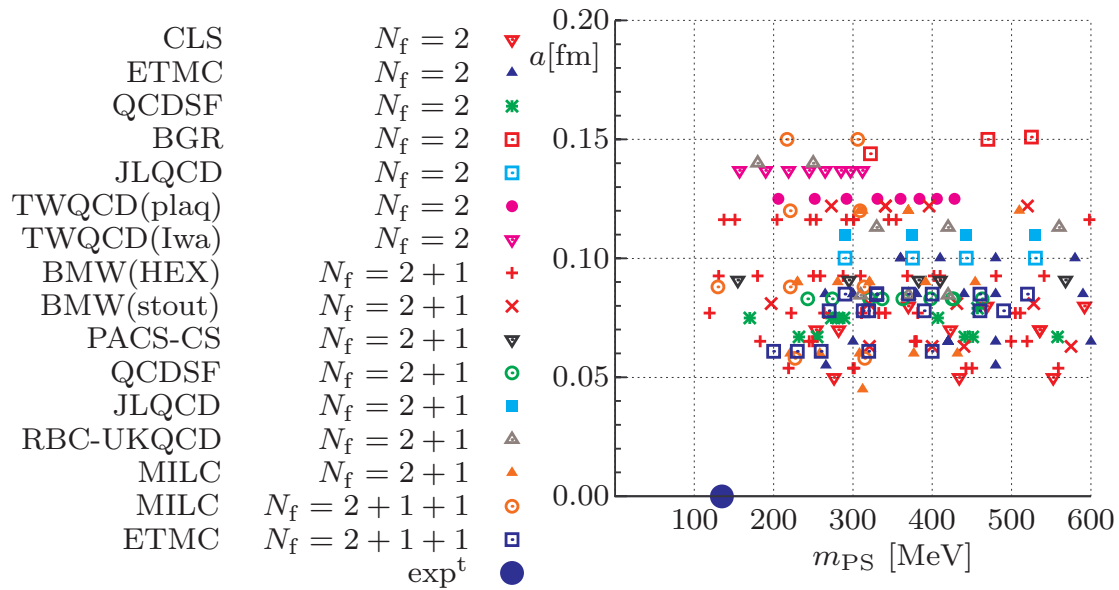


Releasing the quarks: 2 flavours



Simulation landscape

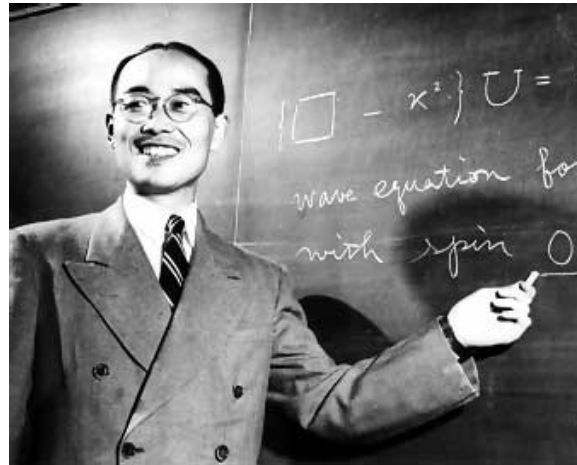
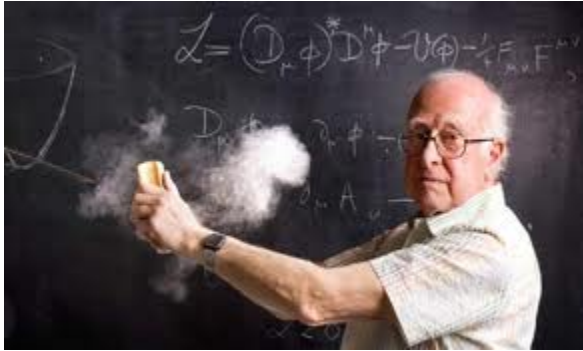
(thanks to G. Herdoiza)



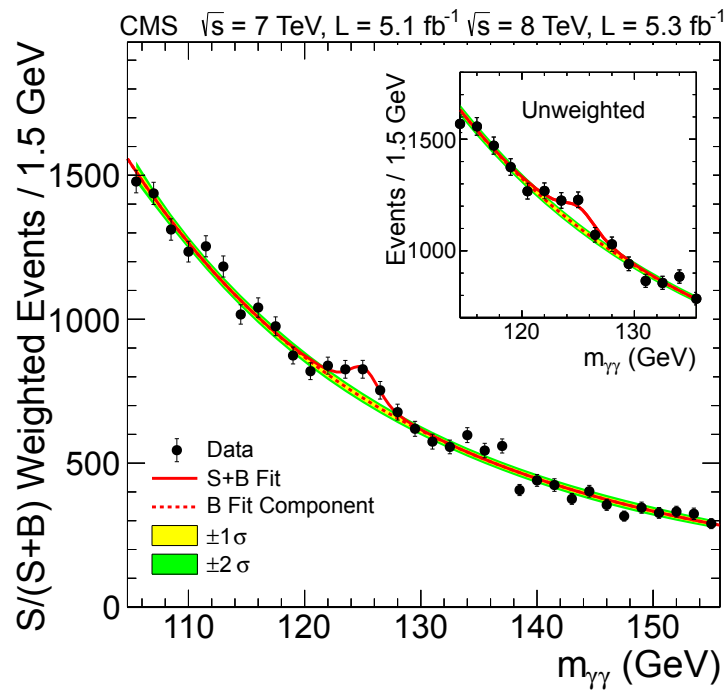




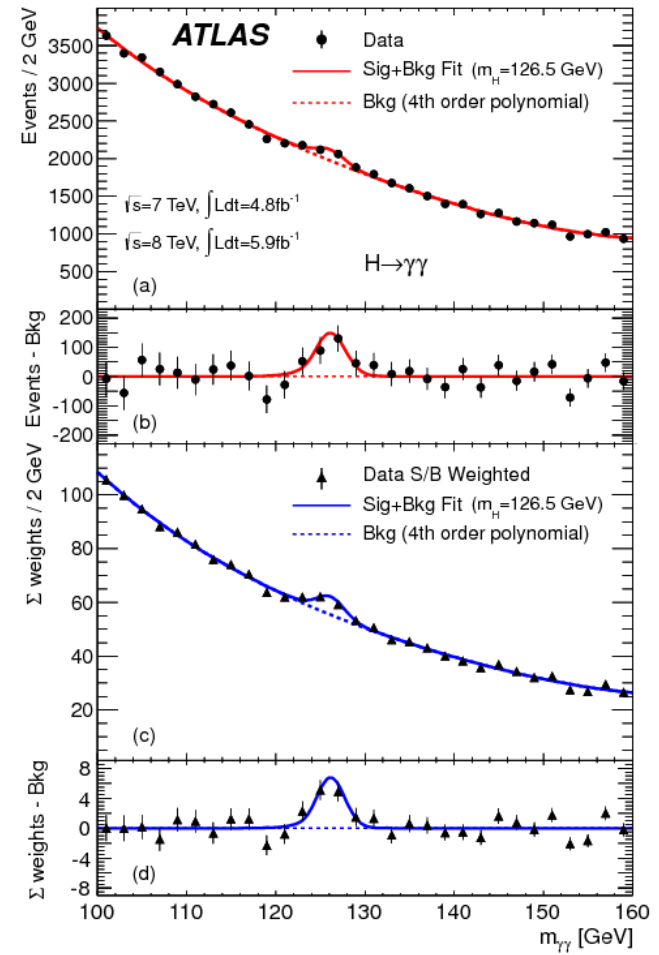
Higgs-Yukawa sector on the lattice



The evidence for a scalar particle at the LHC



CMS



ATLAS

The Higgs-Yukawa sector of the standard model

- the scalar theory

$$L_\varphi[\varphi] = \frac{1}{2}\partial_\mu\varphi_x^\dagger\partial_\mu\varphi_x + \frac{1}{2}m_0^2\varphi_x^\dagger\varphi_x + \lambda(\varphi_x^\dagger\varphi_x)^2$$

- the fermionic and Yukawa parts

$$(L_F + L_Y)[\bar{\psi}, \psi] = \bar{\psi}i\gamma_\mu\partial_\mu\psi + y_b(\bar{t}, \bar{b})_L\varphi b_R + y_t(\bar{t}, \bar{b})_L\tilde{\varphi}t_R + c.c.$$

exact $SU(2)_L$ chiral symmetry: $\gamma_5[L_F + L_Y] + [L_F + L_Y]\gamma_5 = 0$

$$\psi \rightarrow P_+\psi + \Omega_L P_-\psi, \bar{\psi} \rightarrow \bar{\psi}P_+\Omega_L^\dagger + \bar{\psi}P_-,$$

$$\phi \rightarrow \phi\Omega_L^\dagger, \phi^\dagger \rightarrow \Omega_L\phi^\dagger.$$

with $\Omega_L \in SU(2)$,

projectors: $P_\pm = \frac{1 \pm \gamma_5}{2}$

Chiral invariant Higgs-Yukawa lattice action (Lüscher)

- the lattice fermionic and Yukawa parts

$$(L_F + L_Y)[\bar{\psi}, \psi] = \bar{\psi} D_{\text{ov}} \psi + y_b (\bar{t}, \bar{b})_L \varphi b_R + y_t (\bar{t}, \bar{b})_L \tilde{\varphi} t_R + c.c.$$

- change from continuum:

$$- i\gamma_\mu \partial_\mu \rightarrow D_{\text{ov}}$$

$$- P_\pm = \frac{1 \pm \gamma_5}{2} \rightarrow \hat{P}_\pm = \frac{1 \pm \hat{\gamma}_5}{2}, \hat{\gamma}_5 = \gamma_5 (1 - aD_{\text{ov}})$$

- exact *lattice* $SU(2)_L$ chiral symmetry: $\gamma_5 D_{\text{ov}} + D_{\text{ov}} \gamma_5 = aD_{\text{ov}} \gamma_5 D_{\text{ov}}$

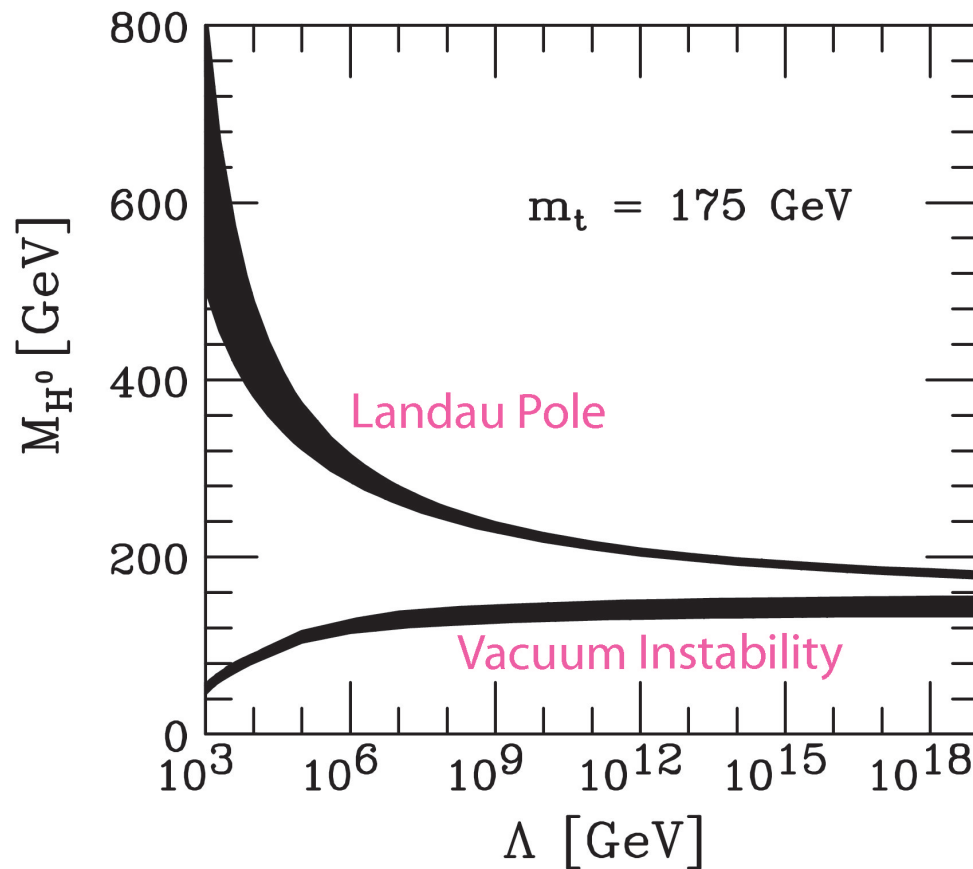
Ginsparg-Wilson relation overlap operator D_{ov} Neuberger

$$\psi \rightarrow \hat{P}_+ \psi + \Omega_L \hat{P}_- \psi, \bar{\psi} \rightarrow \bar{\psi} P_+ \Omega_L^\dagger + \bar{\psi} P_-$$

$$\phi \rightarrow \phi \Omega_L^\dagger, \phi^\dagger \rightarrow \Omega_L \phi^\dagger.$$

with $\Omega_L \in SU(2)$,

Theoretical bounds on the Higgs boson mass



- upper bound from triviality
- lower bound from vacuum instability

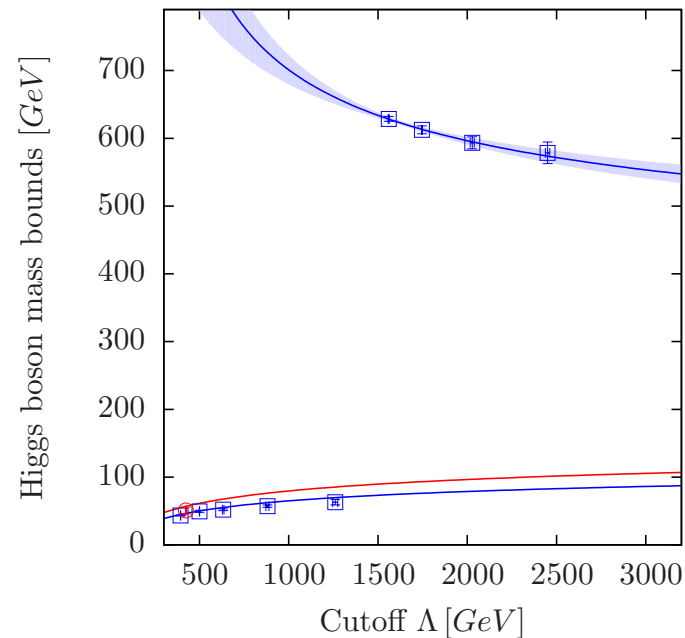
unanswered questions

- upper bound:
 - coupling becomes strong, unclear whether perturbation theory is valid
 - lower bound:
 - is vacuum instability an artefact of perturbation theory?
 - effects of possible very heavy fermions
- ⇒ would like to have a first principles, non-perturbative calculation → lattice

Lower and upper Higgs boson mass bounds

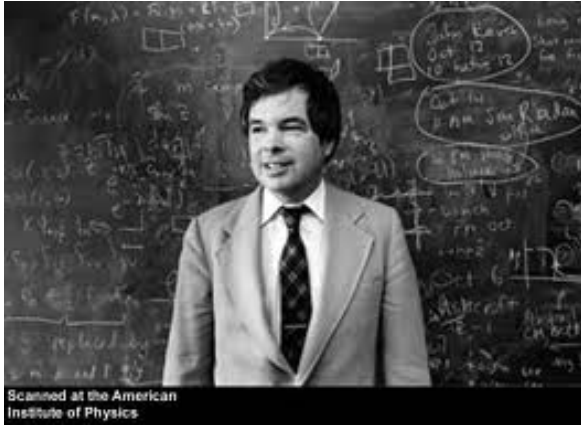
(J. Bulava, P. Gerhold, J. Kallarackal, A. Nagy, K.J.)

- cut-off dependence of lower and upper bounds
- allowed range of Higgs boson mass:
 $50\text{GeV} < m_H < 650\text{GeV}$ at cut-off $\Lambda = 1.5\text{TeV}$



- When does experimental scalar boson mass cut the lower bound? (in progress)

Quantum Chromodynamics on the lattice



Why Perturbation Theory fails for the Strong Interaction

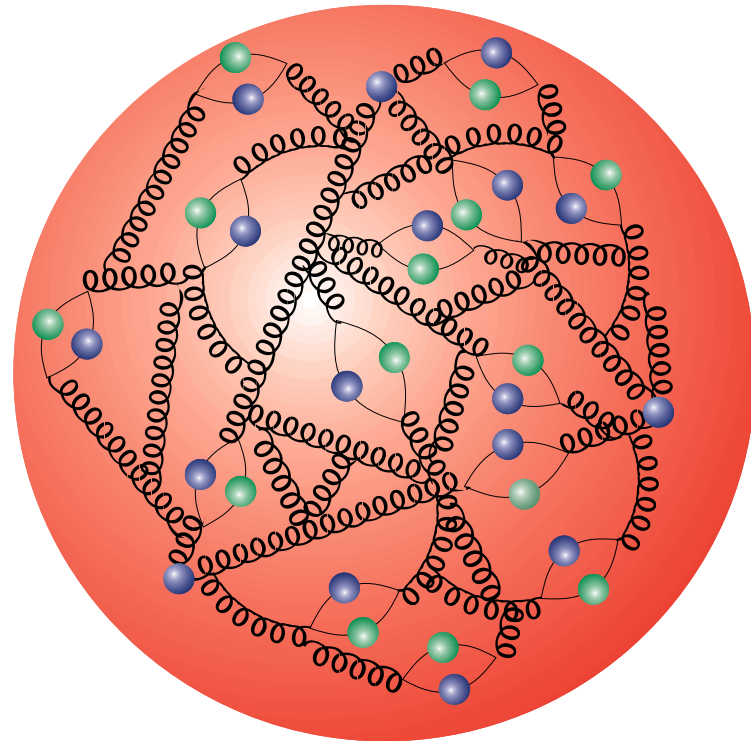
- situation becomes incredibly complicated

- value of the coupling (expansion parameter)
 $\alpha_{\text{strong}}(1\text{fm}) \approx 1$

⇒ need different (“exact”) method

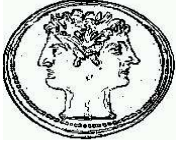
⇒ has to be non-perturbative

- Wilson’s Proposal: Lattice Quantum Chromodynamics



Lattice Gauge Theory had to be invented

→ QuantumChromoDynamics

asymptotic freedom		confinement
distances $\ll 1\text{fm}$		distances $\gtrsim 1\text{fm}$
world of quarks and gluons		world of hadrons and glue balls
perturbative description		non-perturbative methods

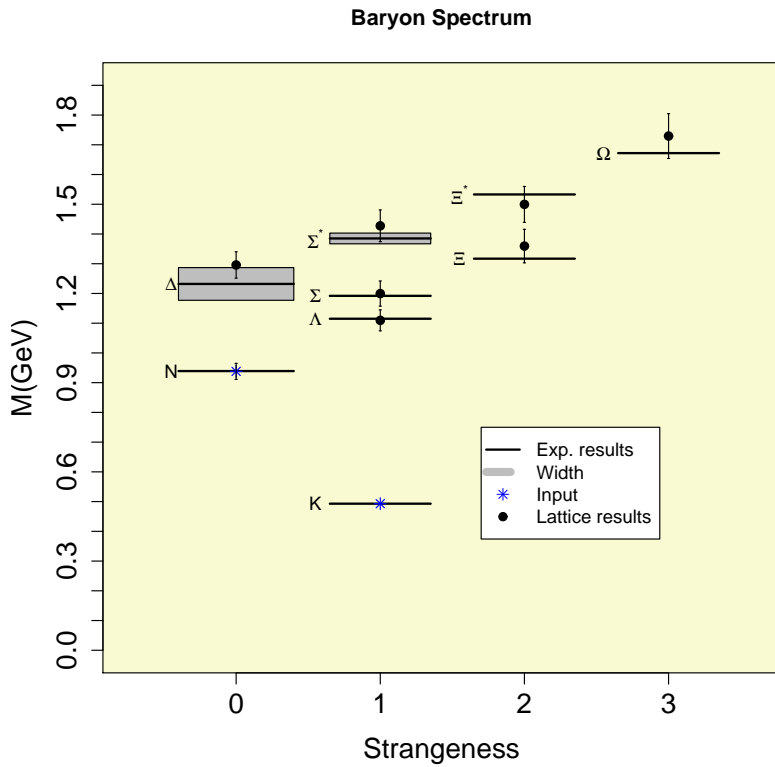
Unfortunately, it is not known yet whether the quarks in quantum chromodynamics actually form the required bound states. To establish whether these bound states exist one must solve a strong coupling problem and present methods for solving field theories don't work for strong coupling.

Wilson, Cargese Lecture notes 1976

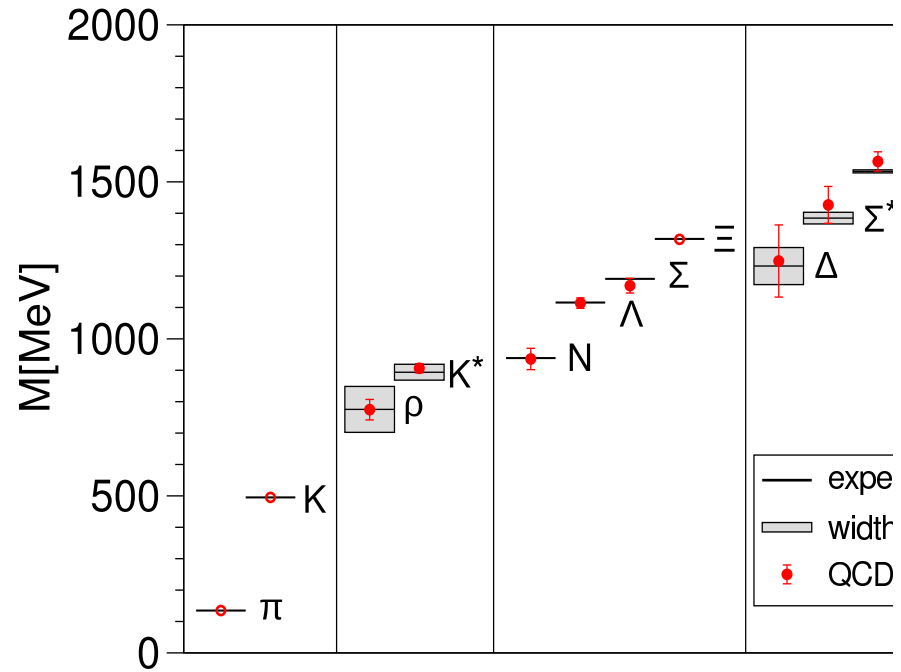
The lattice QCD benchmark calculation: the spectrum

ETMC ($N_f = 2$), BMW ($N_f = 2 + 1$)

progress in lattice QCD: **Hadron Spectrum**



$N_f = 2$



$N_f = 2 + 1$

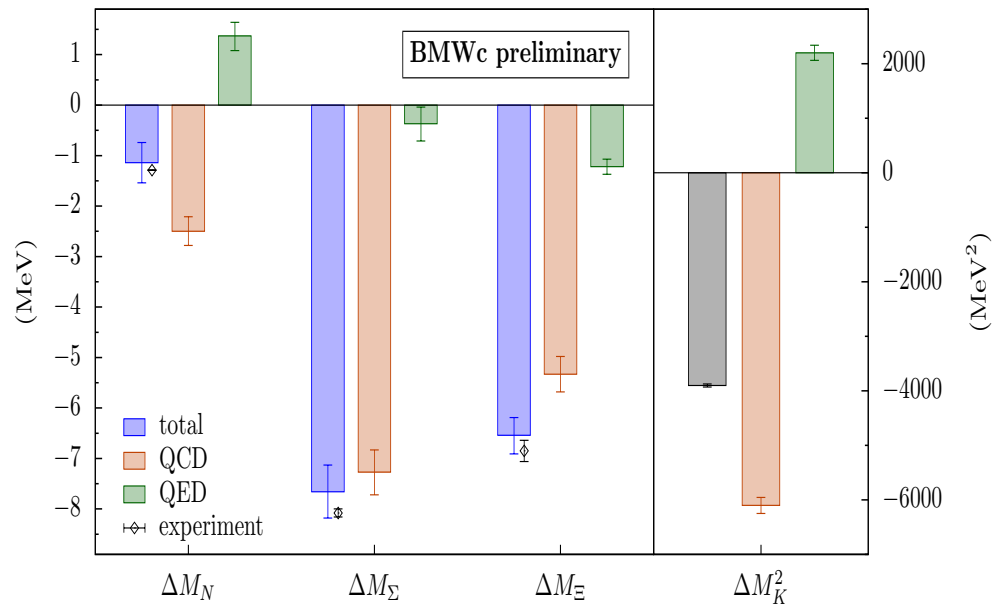
The mass splitting of baryons

(BMW collaboration)

progress in lattice QCD ... and even **Mass splitting**

inclusion of

- isospin-splitting
- (quenched) electromagnetism



→ proton-neutron mass difference from lattice computations

The spin of the electron

- electron carries spin \vec{S}

⇒ magnetic moment $\vec{\mu}_m = -g_e \mu_0 \vec{S}$
 $\mu_0 = e/4m_e$, e electric charge, m_e electron mass

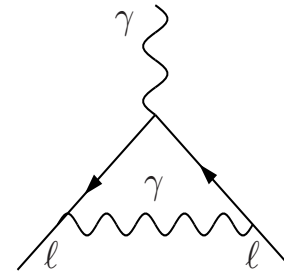
g_e : gyro-magnetic ratio of electron, $g_e = 2$ (Dirac)

- quantum fluctuations

⇒ *anomalous magnetic moment* $a_e = \frac{g_e - 2}{2}$

$g_e = 2.00232$ theory (Schwinger, 1948)

$g_e = 2.00238(10)$ experiment (Foley, 1948)



anomalous magnetic moment of muon a_μ

- nature has decided to have (at least) three families

electron $m_e = 0.511\text{MeV}$, **muon** $m_\mu = 105.7\text{MeV}$, **tau** $m_\tau = 1777\text{MeV}$

- muon anomalous magnetic moment

$$a_\mu^{\text{exp}} = 1.16592080(63) \times 10^{-3}$$

$$a_\mu^{\text{theory}} = 1.16591790(65) \times 10^{-3}$$

- tension between experiment and theory

$$a_\mu^{\text{exp}} - a_\mu^{\text{th}} = 2.90(91) \times 10^{-9}$$

\Rightarrow larger than 3σ discrepancy

- uncertainty in theoretical calculation?
- signs of new physics?

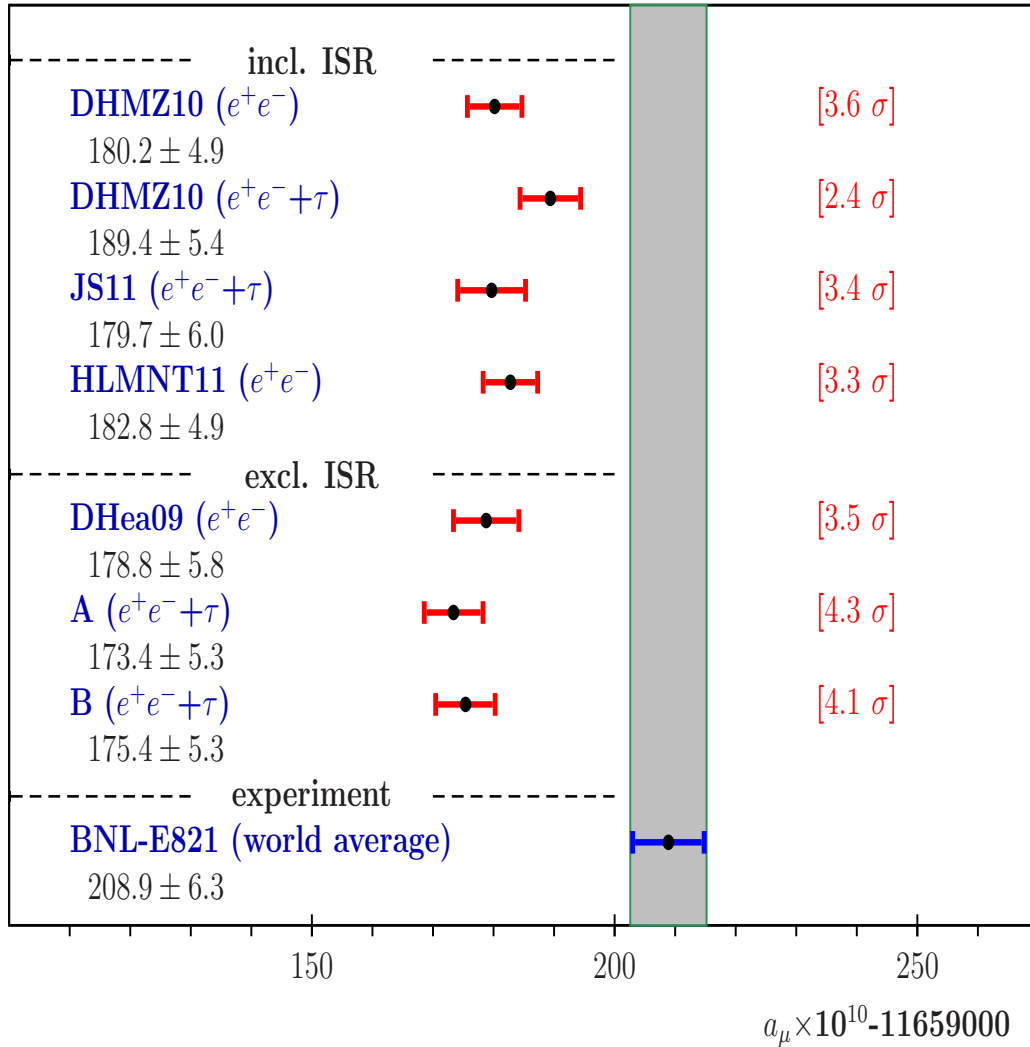
- $\delta(a_l^{\text{newphysics}}) = m_{\text{lepton}}^2 / M_{\text{newphysics}}^2$

since $m_\mu \approx 2 \cdot 10^4 m_e$: a_μ much more sensitive to new physics

- a_τ experimentally hard to measure

Muon magnetic moment: a tension between theory and experiment

→ signs of new physics?



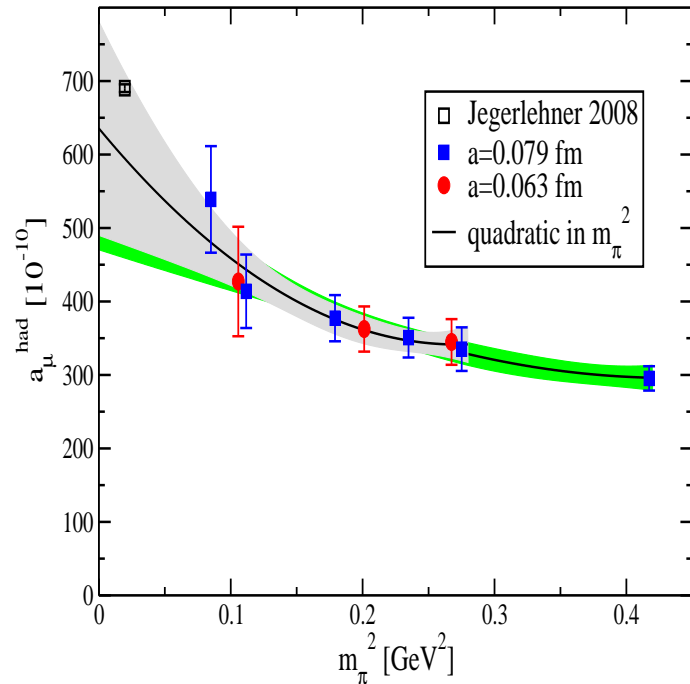
latest analysis

(Benayoun, David, DelBuono,
Jegerlehner)

larger than 4σ discrepancy

Do we control hadronic vacuum polarisation?

(Xu Feng, Dru Renner, Marcus Petschlies, K.J.; Lattice 2010)



• experiment: $a_{\mu, N_f=2}^{\text{hvp,exp}} = 5.66(05)10^{-8}$

• lattice: $a_{\mu, N_f=2}^{\text{hvp,old}} = 2.95(45)10^{-8}$

(numbers are scaled to $N_f = 4$ in plot)

→ misses the experimental value

→ order of magnitude larger error

- have used different volumes
- have used different values of lattice spacing

Different extrapolation to the physical point

lattice: simulations at unphysical quark masses, demand only

$$\lim_{m_{\text{PS}} \rightarrow m_{\pi}} a_l^{\text{hvp,latt}} = a_l^{\text{hvp,phys}}$$

⇒ flexibility to define $a_l^{\text{hvp,latt}}$

standard definitions in the continuum

$$a_l^{\text{hvp}} = \alpha^2 \int_0^{\infty} dQ^2 \frac{1}{Q^2} \omega(r) \Pi_R(Q^2)$$

$$\Pi_R(Q^2) = \Pi(Q^2) - \Pi(0)$$

$$\omega(r) = \frac{64}{r^2 (1 + \sqrt{1 + 4/r})^4 \sqrt{1 + 4/r}}$$

with $r = Q^2/m_l^2$

Redefinition of $a_l^{\text{hvp,latt}}$

redefinition of r for lattice computations

$$r_{\text{latt}} = Q^2 \cdot \frac{H^{\text{phys}}}{H}$$

choices

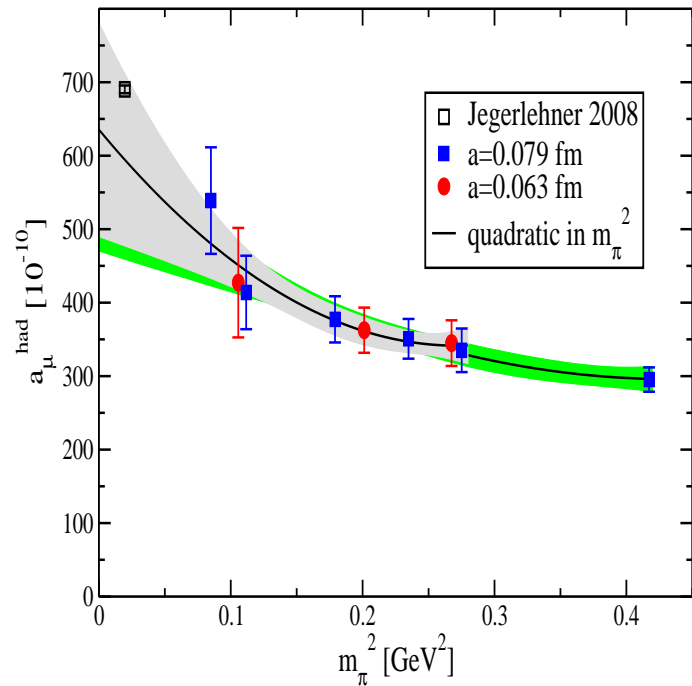
- r_1 : $H = 1$; $H^{\text{phys}} = 1/m_l^2$
- r_2 : $H = m_V^2(m_{\text{PS}})$; $H^{\text{phys}} = m_\rho^2/m_l^2$
- r_3 : $H = f_V^2(m_{\text{PS}})$; $H^{\text{phys}} = f_\rho^2/m_l^2$

each definition of r will show a different dependence on m_{PS} but agree *by construction* at the physical point

- for $m_\mu^2/m_\rho^2 \ll 1$: $a_\mu^{\text{hvp}} = \frac{4}{3}\alpha^2 g_\rho^2 m_\mu^2/m_\rho^2$

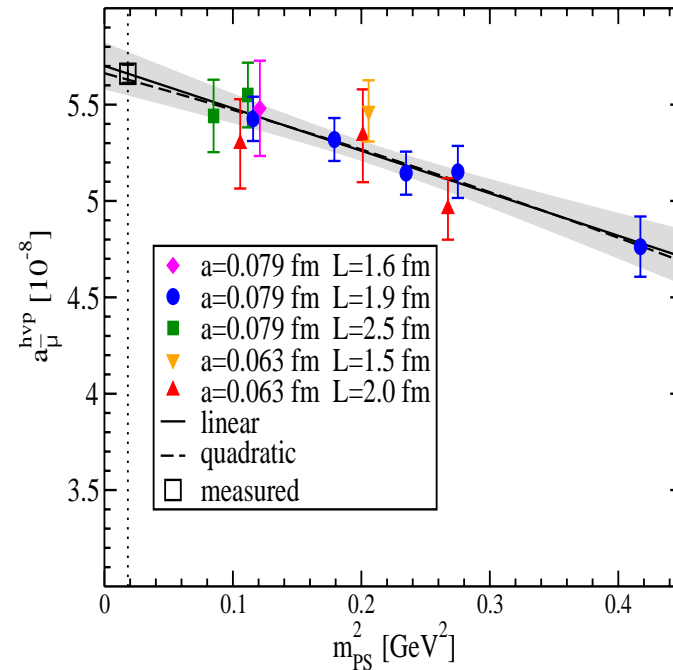
Progress: development of new, improved method

(X. Feng, M. Petschlies, D. Renner, K.J.)



standard method

old: $a_{\mu, N_f=2}^{\text{hvp,old}} = 2.95(45)10^{-8}$



improved method

new: $a_{\mu, N_f=2}^{\text{hvp,new}} = 5.66(15)10^{-8}$

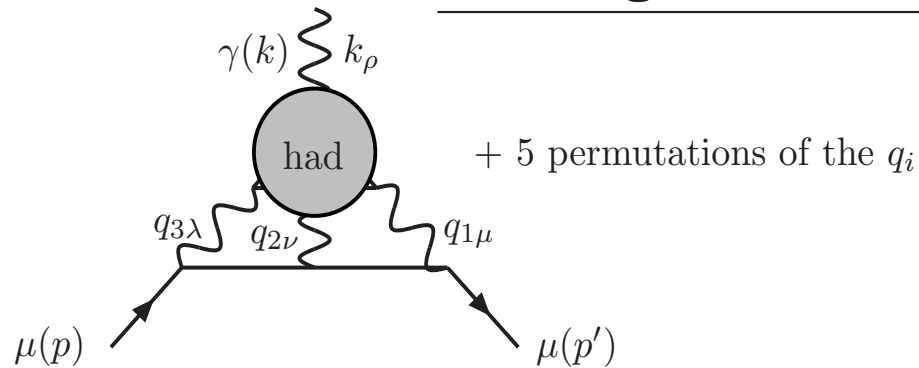
- experimental value: $a_{\mu, N_f=2}^{\text{hvp,exp}} = 5.66(05)10^{-8}$
- different volumes and lattice spacings, included dis-connected contributions
- many groups: JLQCD, Mainz, Brookhaven
- ultimate goal: direct calculation at physical point

WARNING



**CHALLENGES
AHEAD**

Challenge I: next, α_s^3 , contribution



light-by-light scattering

involves 4-point function

$$\Pi_{\mu\nu\alpha\beta}(q_1, q_2, q_3) = \int_{xyz} e^{iq_1 \cdot x + iq_2 \cdot y + iq_3 \cdot z} \langle j_\mu(0) j_\nu(x) j_\alpha(y) j_\beta(z) \rangle$$

j_μ electromagnetic quark current

$$j_\mu = \frac{2}{3} \bar{u} \gamma_\mu u - \frac{1}{3} \bar{d} \gamma_\mu d - \frac{1}{3} \bar{s} \gamma_\mu s + \frac{2}{3} \bar{c} \gamma_\mu c$$

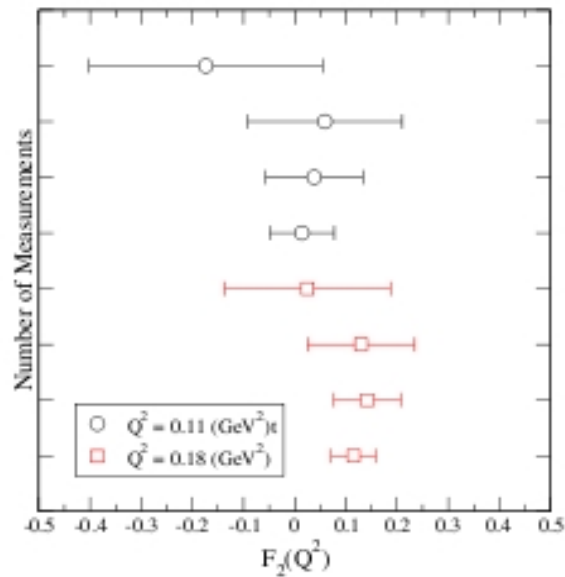
- need $O(V^3)$ momenta
- in turn: $O(V^3)$ “inversions”

\Rightarrow direct calculations not possible

A first attempt

(T. Blum, T. Izubuchi and collaborators)

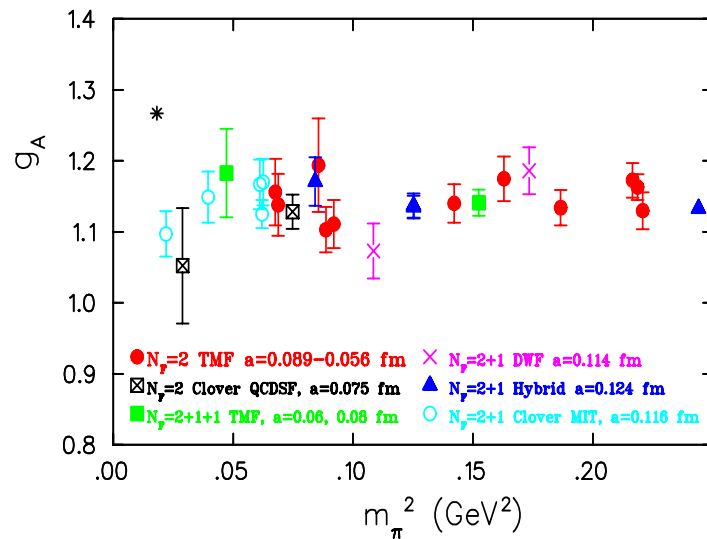
- include electromagnetism in simulations
- problem reduces to difference of 3-point functions



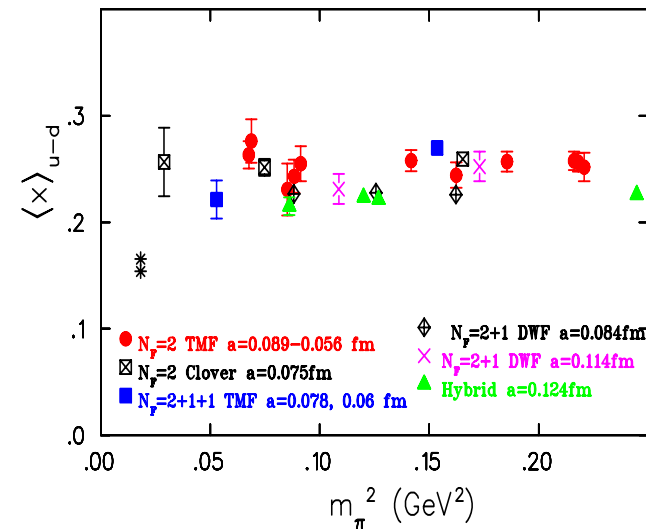
- presently unclear, whether method will be sufficiently precise

Challenge II: hadron structure

- the puzzle with hadron structure



the axial charge



average momentum quark in proton

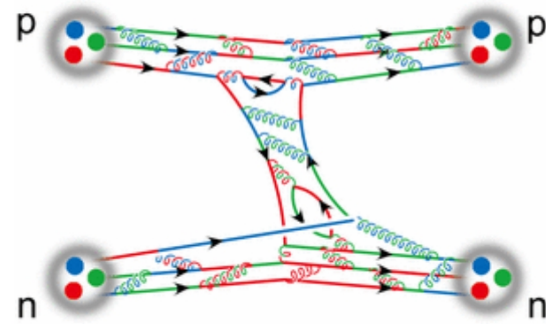
- misses experimental/phenomenological values

⇒ need simulations at physical point

Simulation at physical pion mass

- Lattice spacing: $a = 0.1\text{fm}$
- Pion mass: $m_\pi = 140\text{MeV}$
- Suppression of finite size effects: $L \cdot m_\pi > 5$
- Requirement
 - $L \approx 5\text{fm} \rightarrow 48^3 \cdot 96$ lattice (← present standard)
 - for $a = 0.05\text{fm} \rightarrow 96^3 \cdot 192$ lattice
 - grows of simulation cost $\propto a^{-6}$

Nuclear physics from Lattice QCD



start with Schrödinger equation

$$[H_0 + V(x)] \phi_k(x) = \epsilon_k \phi(x)_k$$

$$\epsilon_k = \frac{k^2}{2\mu} ; \quad \mu = m_N/2 ; \quad H_0 = \frac{-\nabla^2}{2\mu}$$

Reversing this: knowing wave function \rightarrow compute potential

$$[\epsilon_k - H_0] \phi_k(x) = \int d^3y V(x, y) \phi_k(y)$$

Wavefunction from the lattice

$$\phi_k(r) = \langle 0 | N(x+r) N(x) | N N W_k \rangle$$

$$W_k = \sqrt{k^2 + m_N^2}$$

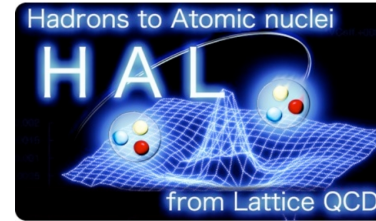
partial wave in infinite volume:

$$\phi_k^l \rightarrow A_l \frac{\sin(kt - l\pi/2 + \delta_l(k))}{kr} \text{ for } r \rightarrow \infty$$

Strategy:

- compute wave function within lattice QCD in finite volume
- determine potential $U(x)$ in finite volume
- use this potential to solve Schrödinger equation in infinite volume
- determine scattering phase or binding energy

⇒ study nuclear physics, neutron stars, supernovae, ...

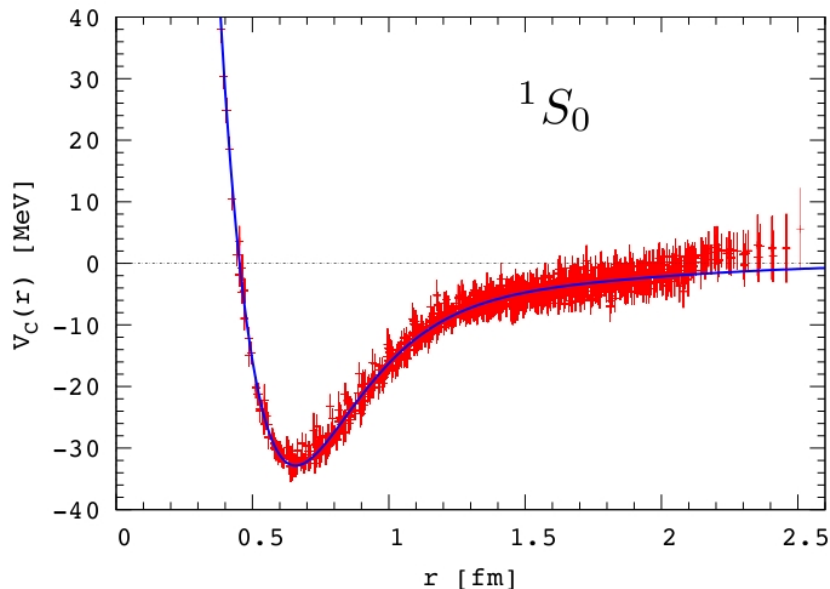


Nuclear physics from Lattice QCD

(Sinya Aoki (U. Tsukuba) Bruno Charron (U. Tokyo)
Takumi Doi (Riken) Tetsuo Hatsuda (Riken/U. Tokyo)

Yoichi Ikeda (TIT) Takashi Inoue (Nihon U.) Noriyoshi Ishii (U. Tsukuba) Keiko Murano (Riken)
Hidekatsu Nemura (U. Tsukuba) Kenji Sasaki (U. Tsukuba) Masanori Yamada (U. Tsukuba))

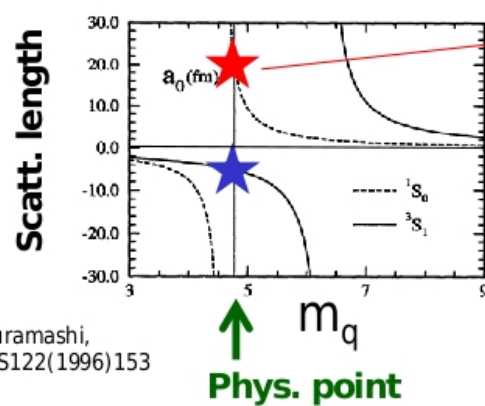
$a=0.09\text{fm}$, $L=2.9\text{fm}$ $m_\pi \simeq 700\text{ MeV}$



(Ishii-Aoki-Hatsuda, PRL90(2007)0022001)

→ paper has been selected as one of 21 papers in Nature Research Highlights 2007.

The challenge and the prospect



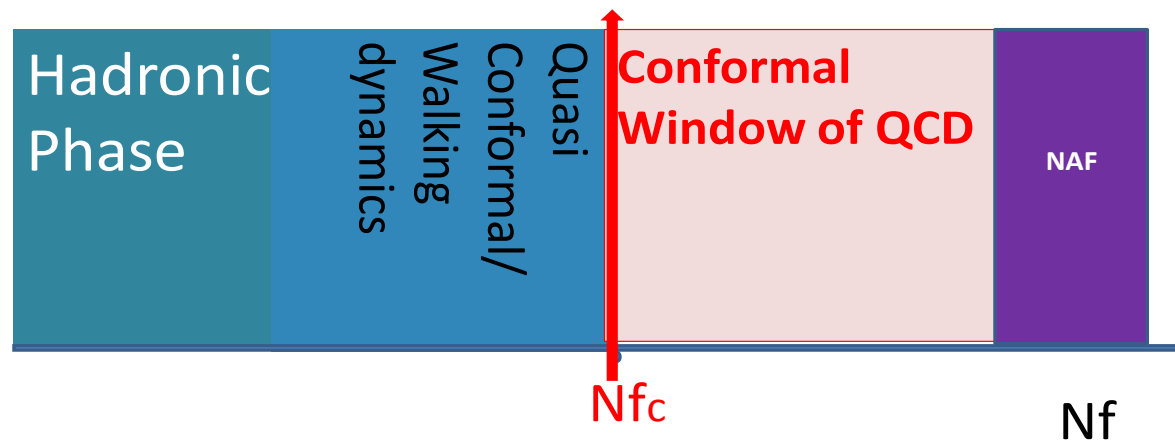
We are here

- in-elastic scattering
- resonances
- extension to weak interactions

⇒ need the **K-Computer**

A new game: looking for the conformal window

QCD with many flavors : Sketchy view of the phase diagram



conformal window: existence of **dilaton**: scalar particle

Higgs boson imposter?

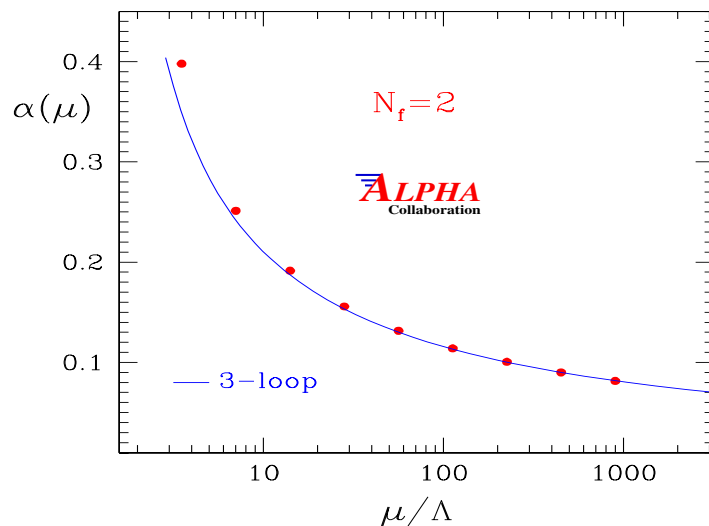
Scale dependence of coupling

$$\mu \frac{\partial}{\partial \mu} \bar{g}^2(\mu) \equiv \beta(\bar{g}^2(\mu)) = \frac{2}{4\pi^2} \left(11 - \frac{2}{3} N_f \right) + \dots$$

- for $N_f > 16$: β -function changes sign \Rightarrow new fixed point



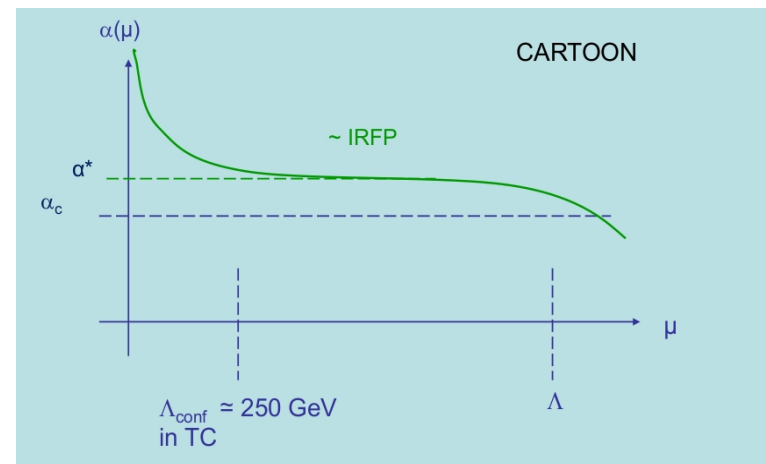
QCD: running coupling



determine “running”: difficult

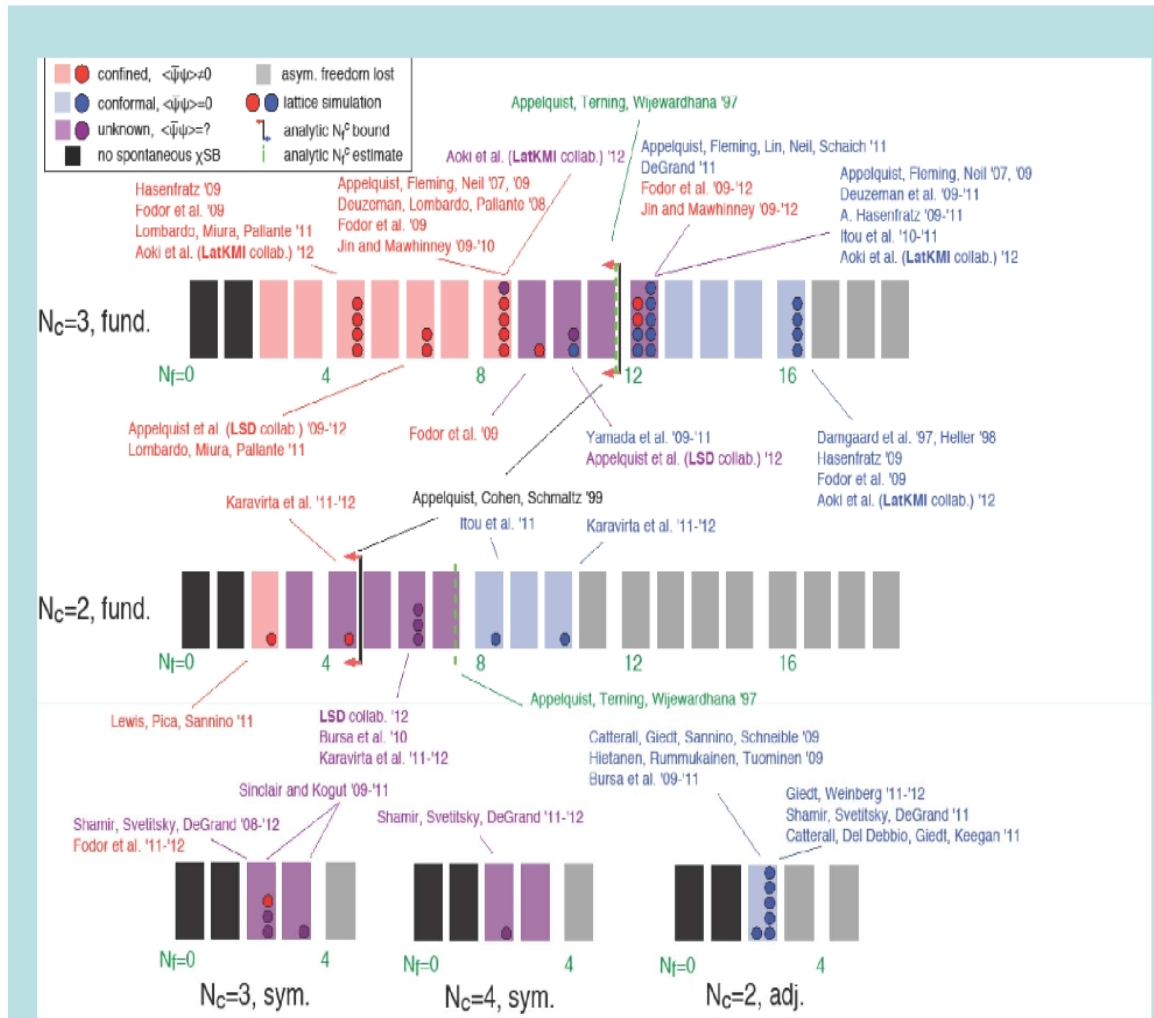


Conformal: walking coupling



\rightarrow identifying “walking” much harder

Large activity in lattice community



The lattice offers much more ...

- Flavour physics, quark masses (*b – quark*), decay constants, α_{strong}
- CKM matrix elements, B_K
- non-zero temperature physics
- topology and chiral symmetry breaking
- charm physics

... and needs this at the physical point



Summary

- Progress in solving QCD with lattice techniques
 - dramatic algorithm improvements
 - new supercomputer architectures
 - theoretical/conceptual developments
- offers to compute many physical quantities, showed
 - non-perturbative Higgs boson mass bounds
 - baryon spectrum
 - leading order hadronic contribution to muon anomalous magnetic moment
- challenges discussed (there are many more)
 - light-by-light contribution
 - nucleon structure puzzle
- simulations in physical situation:
full first two generations at physical quark masses
- new directions
 - nuclear physics
 - conformal theories

